ON THE DEVELOPMENT OF A RISK BASED VERIFICATION PROTOCOL FOR PROCESS MODELLING AND SIMULATION

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ABSTRACT

A risk based procedure for verification of process modelling and simulation (PMS) is presented. The procedure is based on Det Norske Veritas offshore service specification for risk based verification, state-of-the-art methodologies within simulation verification, validation & accreditation, and recognized methods for PMS. The motivation for developing the procedure is the increasing challenges posed by the growing energy demand and climate change which creates an accelerating need for new energy technologies. The procedure is therefore directed towards physical and chemical processes and application with new emerging energy technologies, such as CO_2 capture and CO_2 conversion. Based upon various levels for verification involvement, the procedure describes how to verify subsequent steps in a proposed generalized framework for PMS.

Keywords: verification protocol, risk based, process modelling and simulation

1. INTRODUCTION

To cater the growing energy demand of the world and address the challenges posed by climate change and energy security, new energy processes are being explored and developed. There are several new technical, financial, safety and environmental challenges and risks related to the development of these energy processes.

One of the critical aspects in the development of these new processes is to demonstrate technological feasibility of the concept. To predict and demonstrate technological feasibility, methods such as modelling & simulation and experimental techniques are used. Simulating these new processes often require development of new models and tools. It is important to judge and address the uncertainty and risks associated with their development.

One major uncertainty in the development of models and simulations is the ability to develop them as desired. The objective of the current work is to develop a procedure that addresses this uncertainty and that increases confidence and creates trust for the end user of the simulation results.

1.1. Previous work

Several defence establishments across countries have realized the need for verification, validation and accreditation (VV&A) of simulation of their operation, organization and interests (Australian Department of Defence 2005; Defence Research & Development Canada 2003; United States Department of Defence 2006a). They have published instructions and recommended practices guides for such VV&A's. These guidelines recommend VV&A as a part of modelling and simulation. Use of VV&A is not only considered beneficial but necessary in some cases when use of simulation is critical in decision making.

The US Department of Defence (DoD) published a Recommended Practices Guide for VV&A of modelling and simulation (United States Department of Defence 2001, 2006b). In this Guide, *Verification* means the process of determining that a model implementation and its associated data accurately represent the developer's conceptual description and specifications. Further, *Validation* means the process of determining the degree to which a model and its associated data provide an accurate representation of the real world from the perspective of the intended use of the model. Finally, *Accreditation* is the official certification that a model, a simulation or a federation of models and simulations, and its associated data is acceptable for use for a specific purpose.

The US DoD and the military services have recognized the growing significance of modelling and simulation for many aspects of their operations. The DoD guide describes the interrelated processes that make up VV&A from a number of perspectives. Further, it explains what VV&A is, why it is important to perform, what the key considerations for scoping VV&A are, when it is performed, who the key players are and what are the costs and benefits of such work. The guide by the US DoD is a key document that is referenced and used as a starting point for many others in the literature.

Balci (1997) presented guidelines for conducting VV&A of simulation models. Fifteen guiding principles were introduced to help researcher practitioners and managers better comprehend what VV&A is about. The

VV&A activities were described in the modelling and simulation life cycle. An important principle presented by Balci is that *'VV&A require independence to prevent developer's bias"*.

Preece (2001) provided a critical assessment of the state of the practice in knowledge based V&V. It included a survey of available evidence as to the effectiveness of various V&V techniques in real world knowledge based development projects. For knowledge management practitioners, this paper offers guidance and recommendations for the use of V&V techniques. For researchers in knowledge management, the paper points to the areas where further work needs to be done in developing more effective V&V techniques.

Sargent (2007) discussed the different approaches to deciding model validity. Further, various validation techniques were defined and a recommended procedure for model validation was presented. V&V of simulation was also briefly discussed by Shannon (1998). Sokolowski and Banks (2009) discussed how to perform V&V of simulation including several relevant examples.

The general theory of mathematical modelling and simulation is established, although various descriptions on how to develop and operate a simulation model exist in the literature. Banks (1998) described the steps to guide a model builder in a thorough and sound simulation study. Maria (1997) gave an introduction to modelling and simulation and presented 11 general steps to develop simulation models, designing simulation experiments and performing simulation analyses. Zeigler et al. (2000) described a framework for modelling and simulation by using a different terminology. Hangos and Cameron (2001) described a seven step procedure for process modelling and modelling analysis, directed at the field of process engineering.

The general procedures by Hangos and Cameron (2001) and those described by Banks (1998) have served as the starting point and simulation framework for the verification protocol in the present work.

1.2. Present work

As the previous section shows, VV&A as well as general techniques for process modelling and simulation (PMS) are developed and established by others. The present work extends on these techniques and suggests a risk based verification procedure for PMS that is based on Det Norske Veritas offshore service specification for risk-based verification, state-of-the-art methodologies within V&V, and recognized methods for PMS. The risk based verification concept is described in DNV-OSS-300 (Det Norske Veritas 2004) and is visualized in Fig. 1.

In the present work the definition of *Verification* is: *Confirmation by examination and provision of objective evidence that the specified requirements have been fulfilled. The examination shall be based on information which can be proved true, based on facts obtained through observation, measurement, test or other means.*

Thus, the overall general steps for PMS provide the framework for the verification. The following is addressed in the protocol:

- A generalized procedure for PMS constitutes the framework in which the verification is performed. This framework is based on recognized methods for PMS.
- Description of detailed topics in the verification procedure such as simulation specification, risk assessment and definition of verification involvement by three risk-based verification levels.
- Development and execution of the verification plan that includes a description of how the different steps in the general framework for PMS will be verified for the different levels of verification.

Figure 1: The DNV Risk Based Verification Chain

2. METHODOLOGY

This verification protocol is developed for verification of PMS of physical and chemical processes. The methodology is based on the general principles in the DNV Offshore Service Specification Risk Based Verification (Det Norske Veritas 2004).

The risk based verification process is described in relation to generally accepted methods for PMS, such as the ones described by Hangos and Cameron (2001) and by Banks (1998). These general methods for PMS have been extended to form a generalized modelling and simulation framework that is used to develop the verification plan as shown in Fig. 2.

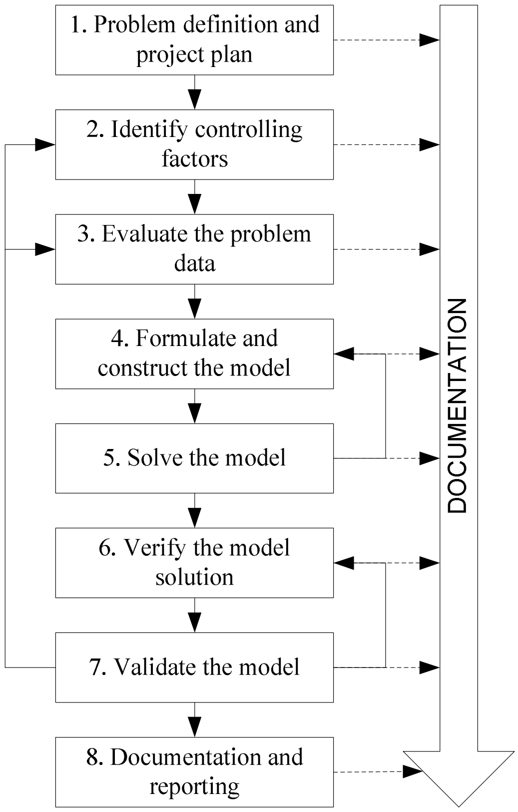

Figure 2: General Steps in Process Modelling and Simulation (PMS)

In this framework, an additional step called '*Documentation*' has been introduced which importance should be emphasized in verification. For detailed description of the key steps in Fig. 2, please refer to Hangos and Cameron (2001) and Banks (1998). A few points regarding the procedure importance are highlighted below.

If the validation results show that the developed model is not suitable for the modelling goal then one has to return to step 2 and perform the sequence again, i.e. it is an iterative procedure. Generally, validation results indicate how to improve the model.

It is recommended to document every action taken in each step of the development of the process model and simulation. This is particularly useful when the process being modelled and simulated is large and complex, and when there are several sub models which constitute the main model.

At the end, a report summarizing all the necessary details about the PMS should be prepared.

3. VERIFICATION OF PROCESS MODELLING AND SIMULATION

This section describes important and detailed aspects related to the verification procedure. This includes planning, simulation specification, risk assessment, determination of verification level and the verification plan of the DNV risk based verification concepts for PMS.

3.1. Simulation planned

This is the starting point for the simulation project and is the decision of the owner. It comprises a general description of the project.

3.2. Simulation specification

At least the following need to be specified at this step:

- Process system description: A process system is a system in which physical and chemical processes that are of interest to a modeller, take place. To define a process system, we need to specify its boundaries, its inputs and outputs and the physio-chemical processes taking place within the system. Process systems are conventionally specified in terms of a flow sheet which defines the boundaries together with inputs and outputs.
- A modelling goal: Specifies what one wants to achieve with the model. The modelling goal has a major impact on the level of detail and on the mathematical form of the model which will be built.
- Acceptance criteria and performance requirements to the simulation.
- Determination of overall verification plan.

3.3. Risk assessment

The risk assessment is a means to determine the required level of verification. The risk assessment includes the identification of hazards, frequencies of occurrence, consequences and risk drivers. It also includes ranking of hazards based on risk evaluation.

The risk can be defined on a general level, for different phases or for detailed elements of the simulation. Risks with PMS are that it fails to give expected results because of aspects such as:

- The model was not built as intended
- The process to be simulated has a degree of novelty and therefore may lead to simplifications in the development of models for the process. These simplifications may distort the results to an extent that these become neither meaningful nor useful in the decision making process.

Consequences of such failure can be the following:

- Incorrect decisions
- Delay in making decisions
- Loss of time, resource and money

3.4. Definition of verification involvement

The level of verification involvement should be differentiated according to the risk to the asset or elements or phases thereof. If the risk to the asset is higher, the level of verification involvement is higher. Conversely, if the risk to the asset is lower, the level of verification activities can be reduced, without any reduction in their effectiveness.

There are three levels of verification of assets, categorized as *low, medium and high*.

Low is the level of verification applied where the risks to the asset are lower than average. For example it has benign contents, it is located in congenial environment conditions, or the contractors are well experienced in the design and construction of similar assets. The level may also be appropriate when the owner (or other parties) performs a large degree of verification or quality assurance work.

With regard to process simulation verification, it is proposed to use the *Low* category of verification in the following situations:

- The process which is simulated is well known and understood, it has no new technical novelty
- The process simulation is carried out as part of the customary design practice, using well known simulation tools by experienced designer/parties.
- The verification of the process simulation is done as part of the modelling and simulation steps described above by the designer. No independent verification is required.

Medium is the level of verification applied where the risks to the asset are average. This is the level of verification which is customary and is applied to the majority of assets. For process simulation verification, it is proposed to use this category of verification in the following situations:

- The process which is simulated has moderate level of technical novelty (technological or application or both) and the process simulation is carried out to predict the performance.
- The process simulation is carried out with well known tools by less experienced users or by well experienced users with relatively new simulation tools.
- The verification of process simulation may require independent verification.

High is the level of verification applied where the risks to the asset is higher than average. For example, it has a highly corrosive content, it is in adverse environmental conditions, it is technically innovative or the contractors are not well experienced in the design and construction of similar assets. This level may also be appropriate when the owner chooses to have a small technical involvement or perform little own verification.

For PMS verification, it is proposed to use the *High* category of verification in the following situations:

- The process which is simulated has high level of technical novelty (application or technological or both) and process simulation is carried out to predict the performance of the process.
- The PMS is carried out by less experienced users with less known simulation tools.
- The owner of the asset (process) is not involved in the process simulation and uses contractors for simulation work.

Independent verification is strongly recommended for High level verification.

3.5. Develop verification plan

This section describes how to develop the *verification plan* including a list of verification activities. The verification plan is developed based on compliance with the general framework for PMS shown in Fig. 2 and the determined verification level for the simulation.

A questionnaire based approach is proposed for the verification in each step. Each question indicates the levels of verification, i.e. the question is addressed. ‘L’, ‘M’ and ‘H’ to denote low level, medium level and high level verification, respectively. Thus, the development of the verification plan should follow procedures as shown in Table 1 to Table 6. For simplicity, only selected parts of the verification plan development are shown in these tables.

3.6. Verification execution

Verification execution is document review, independent analyses, inspection, monitoring, site visits, process audits, technical audits, testing, etc. according to the verification plan.

Information arising from execution should be used to identify continuous improvements to the verification plan.

The purpose of the verification activities is to confirm compliance or non-compliance with the simulation specification.

3.7. Simulation completed

Simulation completed is the end point of any lifecycle phase or phases, which complies with the relevant planned simulation and the simulation specification.

4. APPLICATION OF THE PROTOCOL

The verification protocol described above is applicable to modelling and simulation of physical and chemical processes. The protocol is currently being tested on specific cases that are particularly relevant for the development of environmentally friendly energy processes.

One such process is the electrochemical conversion of CO_2 into a useful product such as formic acid.

Another process is the separation of CO_2 from combustion flue gases by chemical absorption, followed by compression and injection into an underground storage site.

Table 1: Excerpt from Verification of Problem Definition and Project Plan.

Verification activity	*Level*		
	L	*M*	*H*
Problem statement – purpose of simulation, scope of simulation is well defined and documented			
• What is the process to be simulated and why is it being simulated?	x	x	x
• Has the process been described to a sufficient degree of detail and accuracy?	x	x	x
• What are the model characteristics (spatial or lumped, steady-state or dynamic, etc.)?	x	x	x
How was the problem statement formulated?			
• Was it defined by the technology owner?			x
• Has the problem definition been communicated to all relevant parties?			x
• How was the problem definition communication done?			x

Table 2: Excerpt from Verification of Identification of Controlling Factors or Mechanism.

Verification activity	*Level*		
	L	*M*	*H*
Have the processes or phenomena taking place in the system been identified and documented?	x	x	x
Are these processes or phenomena well known and have they been simulated before?		x	x
What are the new aspects of the processes or phenomena taking place in the system, if any?		x	x
Did new aspects of the processes or phenomena require simplifications and assumptions in the development of the simulation?		x	x
Have accuracy and tolerance of the simulation been discussed and agreed?			x

Table 3: Excerpt from Verification of the Data for the Simulation.

Verification activity	*Level*		
	L	*M*	*H*
What is the data used in the simulation?	x	x	x
How reliable is the data?		x	x
What is the precision and uncertainties with the data and what will be the impact of these on the simulation results?			x

Table 4: Excerpt from Verification of Model Solution.

Verification activity	*Level*		
	L	*M*	*H*
Are the outputs from the model as expected?	x	x	x
Has a sensitivity analysis of the output been done?		x	x
In case of high level verification, it may be necessary to perform simulations using two different simulation tools and compare the results.			x
Have the results been discussed with the client and with experts, and agreed and documented?	x	x	x

Table 5: Excerpt from Validation of the Model.

Verification activity	*Level*		
	L	*M*	*H*
Has the model been validated?	x	x	x
How is the model validated?			
• By verifying experimentally the simplifying assumptions		x	x
• By comparing the model behaviour with process behaviour		x	x
• By developing an analytical model for simplified cases and comparing behaviour		x	x
• By comparing with other models using a common problem		x	x
• By comparing the model with available process data		x	x

Table 6: Excerpt from Verification of Documentation.

Verification activity	*Level*		
	L	*M*	*H*
Has all the work been properly documented?	x	x	x
Has the owner reviewed the report and agreed with the report's findings?		x	x

5. DISCUSSION

No specific document on VV&A directed towards process engineering modelling and simulation has so far been identified by the authors. However, the basic steps and procedures for VV&A found in the literature can also be used for VV&A of PMS.

For instance, the principles explained in the VV&A Recommended Practices Guide by the US DoD are generic and can be applied to the verification of PMS to an extent. This guideline also states that 'risk' determines the detail or level of verification along with technical and resource constraints. The DNV risk based verification as described in DNV-OSS-300 (Det Norske Veritas AS 2004) is more explicit on risk classification and associated verification activities than what is presented and discussed by the US DoD and others.

Furthermore, the terminology and steps used in PMS, such as those presented by Hangos and Cameron (2001), are not entirely the same as those discussed in literature in general for modelling and simulation.

Thus, the guidelines by DoD alone will not suffice as a guiding and complete document for the verification of PMS. However, the work by the US DoD has served as a starting point for the present work on writing such a guideline. The various verification and validation techniques described in the US DoD documents are the same as those that are typically employed by DNV during verification, such as audit, review, inspection, walkthrough, HAZID etc.

6. CONCLUSIONS

This work has shown the development of a protocol for risk based verification of process modelling and simulation (PMS). Application of the protocol will address uncertainty and risks associated with the development of PMS and thus provide confidence and trust to the stakeholders.

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Det Norske Veritas (DNV) is an autonomous and independent foundation with the objectives of safeguarding life, property and the environment, at sea and onshore. DNV undertakes classification, certification and other verification and consultancy services relating to quality of ships, offshore units and installations, and onshore industries worldwide, and carries out research in relation to these functions. http://www.dnv.com/.

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